Topological derivative method for bilevel optimization on networks

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Outline

Background

- The networks of distributed parameter systems are used:
  - gas or water transportation modeling and control
  - structural optimization for networks of beams
- Mathematical models: flow characteristics, pipeline geometry, material properties, and interactions with other systems.
- Distributed parameter systems: temperature, pressure, and flow velocity.

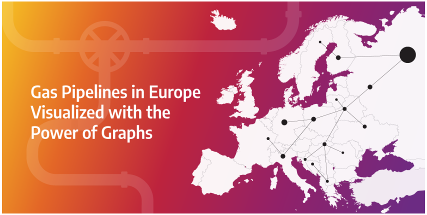

Fig. 1: Illustration for the pipeline in Europe.

Shape Optimization

In shape optimization, a general minimization problem reads

$$J(\Omega) = I(\Omega, u_\Omega) \longrightarrow \inf_{\Omega}$$

where $\Omega \subset \mathbb{R}^n$ is an open set and u_Ω stands for the solution of the state equation for solids or fluids.
There are two methods to determine the descent direction for the gradient method of shape optimization

1. Boundary variations and shape gradients;
2. Topological derivatives and the level set method.

The convergence of the shape gradient flow method for the Kohn-Vogelius functional is shown in two spatial dimensions (P.I. Plotnikov, J.S., JGEA, 2023).

Topological Derivatives for Networks

The topological derivatives for Partial Differential Equations on graphs are introduced by G. Leugering, J.S.

1. The topological derivative of energy functional (no adjoint state) for Timoshenko beams is solved by Ewald Ogiermann (2015).
2. The Steklov-Poincaré operator is employed by J.S., A. Zochowski (2005, Numerische Mathematik) for contact problems of elasticity system in order to separate the singular domain perturbations of topological derivatives from the nonsmooth, unilateral mechanical contact by the technique of domain decomposition.

Shape Functional for Control Problems

In shape optimization of control systems, the minimization problem reads

$$J(\Omega) = I(\Omega, u_\Omega, y_\Omega) \longrightarrow \inf_{\Omega}$$

where $\Omega \subset \mathbb{R}^n$ is an open set and u_Ω stands for the optimal control in Ω, y_Ω the solution in Ω of the state equation for the optimal control.

Shape Functional for Control Problems in Networks

In the case of graphs, we consider the optimal value of the cost for control problem as the shape functional for shape and topology optimization.
Nonlinear state equations are of importance for network optimization.
We consider linear state equations in order to establish the elementary results on topology optimization.

Steklov-Poincaré operator

- In the lecture of Prof. G. Leugering the domain decomposition method for networks was introduced and analysed. In this method, the so-called Steklov-Poincaré operator is employed.
- We use the operator for a modification of the state equation. The small geometric perturbation of the network topology at an interior node is considered. The size of perturbation is governed by small parameter $\varepsilon \to 0^+$. The Steklov-Poincaré operator $\Lambda(\varepsilon)$ **replaces** the geometric perturbation in weak form of the state equation. In this way the properties of solutions to state equations with respect to ε can be analyzed provided the form of $\Lambda(\varepsilon)$ is determined. This approach has already been used for the Lapacian, linear elasticity, and Stokes problem.

Bilevel optimization on networks

- Shape sensitivity analysis is performed for graphs: a single edge, a cross, and the cross with a small cycle.
- Shape functional at the higher level is defined by the optimal value of the cost for control problem.
- Optimal control problem admits the unique local solution determined by the coupled (state and adjoint state) optimality system.
- Both the evolution state equation and the steady state equation are considered for purposes of bilevel optimization.
- The topological derivative of the cost for the steady state equation is introduced and evaluated for the cross with a small cycle.

Optimal control problem in variable domain

- The model includes the state equation and the cost functional.
- The necessary and sufficient optimality conditions are derived in the framework of Lagrangian formalism.
- Another possibility for nonlinear state equations is the Pontryagin's Maximum Principle for combined shape and control problems.
- The optimality system is solved numerically and the optimal value of the cost is evaluated.
- The sensitivity analysis of optimal cost with respect to the shape and topology is performed.

Wave equation for a single edge

- Interval $I_\varepsilon := [0, 1+\varepsilon]$, $|\varepsilon| \leq 0.1$, where ε is the shape parameter
- State equation
$$y_{tt} - y_{xx} = 0, \text{ on } (0, T) \times (0, 1+\varepsilon) \tag{1}$$
- Initial conditions
$$y(0, x) = y^0(x), \; y_t(0, x) = y^1(x) \tag{2}$$
- Boundary conditions
$$y_x(t, 0) = u(t), \; y(t, 1+\varepsilon) = 0 \tag{3}$$
- $u(t)$ is the Neumann control at the boundary $x = 0$

- Tracking type cost functional

$$J(u) = \int_0^T \int_0^{1+\varepsilon} \chi(x)(y_\varepsilon(x) - z(x))^2 dxdt + |u - \zeta|^2_{H^m(0,T)}\,, \tag{4}$$

where $\chi(x)$ is the characteristic function of $[0, 0.9]$, i.e., $\chi(x) = 1$ on $[0, 0.9]$ and $\chi(1-x) = 0$, $m = 2, 3$

- $z = z(x)$, $x \in I = [0, 1+\varepsilon_0]$ and $\zeta \in \mathbb{R}$ are given by the solution of ODE

$$z''(x) = 0 \quad \text{in}\,(0, 1+\varepsilon_0), \quad z'(0) = \zeta, \quad z(1+\varepsilon_0) = 0\,, \tag{5}$$

where $\varepsilon_0 = 0 \in [-0.1, 0.1]$ is fixed.

Coupled system

- Lagrangian functional

$$\mathcal{L}(u, y, p) = \int_0^T \int_0^{1+\varepsilon} (y_{tt} - y_{xx})\, p + J(u). \tag{6}$$

- State equation: $\left\langle \frac{\partial \mathcal{L}}{\partial p}, \eta \right\rangle = 0 \Longrightarrow$ Eq.(1)-Eq.(3)
- Adjoint-state equation: $\left\langle \frac{\partial \mathcal{L}}{\partial y}, \eta \right\rangle = 0 \Longrightarrow$

$$\begin{cases} p_{tt} = p_{xx} + \chi(x)(z - y) \text{ on } [0, T] \times [0, 1+\varepsilon], \\ p(T, x) = 0, \; p_t(T, x) = 0, \; x \in [0, 1+\varepsilon], \\ p_x(t, 0) = 0, \; p(t, 1+\varepsilon) = 0, \; t \in [0, T]. \end{cases} \tag{7}$$

- Optimality condition for $m = 2$: $dJ(u; w) = 0 \Longrightarrow$

$$u \in H^2(0, T): \quad \int_0^T u_{tt} w_{tt} = -\int_0^T p(t, 0) w(t), \quad \forall w(t) \in H^2(0, T). \tag{8}$$

Boundary control on the cross

- Consider the wave equation on a planar graph $G := \{E, V\}$.
- $V = V_B \cup V_J$, (V_B : boundary vertices, V_J : junction vertices)
- Denote $n_{E_i}(P_j)$ by

$$n_{E_i}(P_j) = \begin{cases} -1 \text{ if node } P_j \text{ is the start node of } E_i \\ +1 \text{ if node } P_j \text{ is the end node of } E_i \\ \ \ 0 \text{ otherwise} \end{cases}$$

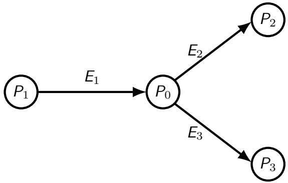

Fig. 2: Tripod directed network.

$$V = \{P_0, P_1, P_2, P_3\},$$
$$E = \{E_1, E_2, E_3\}$$
$$V_B = \{P_1, P_2, P_3\},\ V_J = \{P_0\}$$
$$n_{E_1}(P_1) = n_{E_2}(P_0) = n_{E_3}(P_0) = -1$$
$$n_{E_1}(P_0) = n_{E_2}(P_2) = n_{E_3}(P_3) = 1$$

Transmission Condition

Assume y_i is the state on E_i.

- Continuity Condition

$$y_i(P_j) = y_k(P_j), \forall i, k \in I_E, j \in n_V$$
$$(y_1(P_0) = y_2(P_0) = y_3(P_0))$$

- Kirchhoff Condition

$$\sum_{E_i} \partial_x y_i(P_j) n_{E_i}(P_j) = 0, \forall i \in I_E, j \in n_V$$
$$(\partial_x y_1(P_0) - \partial_x y_2(P_0) - \partial_x y_3(P_0) = 0)$$

where $I_E := \{1, \dots, n_E\}$ and $I_V := \{1, \dots, n_V\}$ denote the set of edge indices and the set of vertex indices, respectively.

- Consider the regular perturbations Ω_ε of the shape Ω of a graph G. $G_\varepsilon := \{E_\varepsilon, V_\varepsilon\}$ with three edges of the length
$$|E_{\varepsilon,1}| = 1 - 2\varepsilon, |E_{\varepsilon,2}| = |E_{\varepsilon,3}| = 1 + \varepsilon.$$
Total length of the graph is constant $|E_{\varepsilon,1}| + |E_{\varepsilon,2}| + |E_{\varepsilon,3}| = 3$.
- The cost functional is defined on the subset $\Omega_0 := \Omega \setminus \overline{\mathcal{O}(P_0)}$ which independent of ε. It means that the small cycle is included in $\mathcal{O}(P_0)$ for all admissible $-c \le \varepsilon \le c$, for some small $c \in \mathbb{R}$.
$$J(u) = \frac{1}{2}\int_0^T \int_\Omega \chi(y - z)^2 + \frac{1}{2}|u|_m^2 .$$

Topological derivative

- The topological derivative method in shape and topology optimization is a new tool that can be used to minimize the shape functionals under the Partial Differential Equations (PDEs) constraints.
- Given the shape functional $\Omega \to J(\Omega)$, the topological derivative at the interior vertex $P_0 \in V$ is defined by the following limit, if the limit exists,

$$\mathcal{J}(P_0) := \lim_{\varepsilon \to 0} \frac{1}{\varepsilon}(J(\Omega_\varepsilon) - J(\Omega)) . \tag{9}$$

The existence of limit in Eq. (9) implies the expansion of the shape functional

$$J(\Omega_\varepsilon) = J(\Omega) + \varepsilon \mathcal{J}(P_0) + o(\varepsilon) . \tag{10}$$

Singular perturbation of the graph at the central vertex by a small cycle

- Consider the cross with six edges of the length $|E_1| = |E_2| = |E_3| = 1 - \varepsilon$, and $|E_4| = |E_5| = |E_6| = \varepsilon$ for $\varepsilon \to 0^+$
- Total length of the graph is constant $|E_1| + |E_2| + |E_3| + |E_4| + |E_5| + |E_6| = 3$
- A boundary control $u(t)$ at vertical P_1, i.e., $\dfrac{\partial y_1}{\partial x}(t, 0) = u(t)$

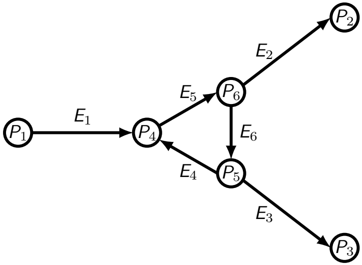

Fig. 3: Tripod directed network with a cycle.

- Steady-state equation:

$$\begin{cases} -z_i'' = 0, x \in [0, L_i] \\ z_1'(0) = \zeta, z_2(L_2) = z_3(L_3) = 0 \\ z_i(P_j) = z_k(P_j), \forall i, k \in I_E, j \in n_V (\text{Continuity Condition}) \\ \sum_{E_i} z_i'(P_j) n_{E_i}(P_j) = 0, \forall i \in I_E, j \in n_V (\text{Kirchhoff Condition}) \end{cases} \quad (11)$$

- Optimality condition: optimal control $u(t) := \mathcal{L}[p](t)$

$$u \in H^2(0,T): \quad \int_0^T u_{tt} w_{tt} = -\int_0^T p(t,0) w(t), \quad \forall w(t) \in H^2(0,T) \quad (12)$$

$$u(0) = u(T) = \zeta, \;\; u_t(0) = u_t(T) = 0.$$

- State equation

$$\begin{cases} (y_i)_{tt} - (y_i)_{xx} = 0, t \in [0,T], x \in [0, L_i], \forall i \in I_E \\ y_i(0,x) = y_{i,0}(x), \;\; (y_i)_t(0,x) = y_1(x), \\ (y_1)'(t,0) = \mathcal{L}(t), \;\; (y_2)(t, L_2) = 0, \;\; (y_3)(t, L_3) = 0, \\ y_i(t, P_j) = y_k(t, P_j), \forall i, k \in I_E, j \in n_V \\ \sum_{E_i} y_i'(t, P_j) n_{E_i}(P_j) = 0, \forall i \in I_E, j \in n_V \end{cases} \quad (13)$$

- Adjoint equation

$$\begin{cases} (p_i)_{tt} = (p_i)_{xx} + \chi(z_i - y_i) \text{ in } t \in [0, T], x \in [0, L_i],\ i \in I_E \\ p_i(T, x) = 0,\ (p_i)_t(T, x) = 0, \\ (p_1)'(t, 0) = 0,\ (p_2)(t, L_2) = 0,\ (p_3)(t, L_3) = 0, \\ p_i(t, P_j) = p_k(t, P_j), \forall i, k \in I_E, j \in n_V \\ \sum_{E_i} p_i'(t, P_j) n_{E_i}(P_j) = 0, \forall i \in I_E, j \in n_V. \end{cases} \tag{14}$$

Algorithm 1: Fixed point algorithm

1. Choose u^0 ;
2. **For** $i = 1$ until satisfied ;
   a. solve state equation for y_i ;
   b. solve adjoint equation for p_i ;
   c. solve optimal condition for u_i ;
3. Terminate with the (approximate) fixed point $\hat{u}, \hat{y}, \hat{p}$.

Numerical Scheme

- The weak formulation of the state equation on the graph:

$$y := y_\varepsilon \in V_\varepsilon := V(\Omega_\varepsilon)$$

$$\begin{cases} (y_{tt}, \varphi)_{L^2(\Omega_\varepsilon)} + a_\varepsilon(y, \varphi) = (u(t), \varphi_1), \quad \forall \varphi \in V_\varepsilon \\ y(0,x) = y_0(x), y_t(0,x) = y_1(x), \end{cases} \tag{15}$$

where $a_\varepsilon(y, \varphi) = \sum_{i=1}^{n_E} \int_0^{L_i} y_i' \varphi_i' dx$ is bilinear form and $\varphi_1(x)$ is the test function on edge E_1.

- The space V is defined as

$$V = \left\{ \varphi = (\varphi_1, \cdots, \varphi_{n_E}) \mid \varphi_i \in H^2(0, L_i), i = 1, \cdots, n_E, \varphi_i(P_i) = 0, i = 2, 3, \right.$$
$$\left. \text{continuity and Kirchhoff conditions at the inner vertices } P_j \in V_J \right\},$$

Numerical discretization

- Time: Finite-difference

$$
\begin{aligned}
y_t(t,x) &\approx \frac{y(t+\Delta t,x)-y(t-\Delta t,x)}{2\Delta t},\\
y_{tt}(t,x) &\approx \frac{y(t+\Delta t,x)-2y(t,x)+y(t-\Delta t,x)}{(\Delta t)^2},
\end{aligned}
\tag{16}
$$

where Δt is the time step.

- Space: Hermite finite element

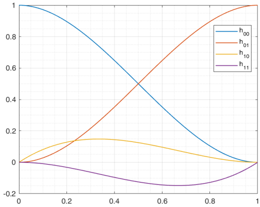

Fig. 4: The four Hermite basis functions on the unit interval $[0, 1]$.

Numerical results

Set $\zeta = 1$, $T = 1, \varepsilon = 0.5, \varepsilon_0 = 0.5$.

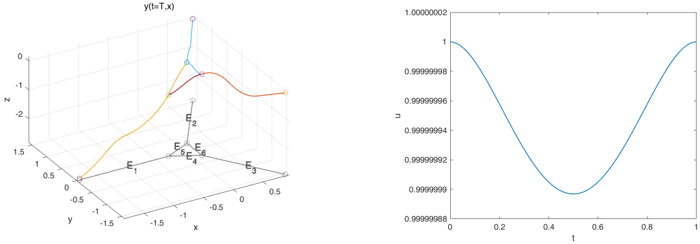

Fig. 5: Final state $y(T, x)$(left) and optimal control(right) for wave equation.

Steady state boundary control problem

- The state equation on $G = \{V, E\}$ is defined in weak form by
$$y \in H : a(y, \phi) = \langle L(u), \phi \rangle \quad \forall \phi \in H,$$
$$H = \left\{\phi, \phi_i' \in L^2\left(0, L_i\right),\ \phi_2(0) = \phi_3(0) = 0,\ \text{continuity at interior vertices.}\ \right\} \tag{17}$$
- $G = G^0 \cup G_\varepsilon$, $|E_{\varepsilon,1}| = |E_{\varepsilon,2}| = |E_{\varepsilon,3}| = \varepsilon_{\max} - \varepsilon = 1 - \varepsilon$

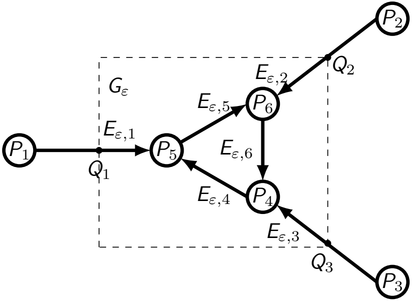

Fig. 6: Tripod directed network with a cycle with domain decomposition.

Steklov-Poincaré operator

Definition 1 (Steklov-Poincaré operator)

A Steklov-Poincaré operator maps the values of Dirichlet boundary condition on the boundary of the graph to the values of Neumann boundary condition for the solution of an elliptic partial differential equation on the graph.

Definition 2 (Dirichlet-to-Neumann operator)

Let us consider the nonhomogeneous Dirichlet boundary value problem with the data $a \in \mathbb{R}^n$. For the unique solution, we look for the Neumann boundary conditions $b = -\Lambda a \in \mathbb{R}^n$, the Steklov-Poincaré operator, in this case, is given by a matrix Λ.

- Determine on G_ε the Dirichlet-to-Neumann nonlocal operator given by a matrix $(\Lambda_\varepsilon)_{3\times 3}$ by the solution for the boundary conditions

$$w_i(0) = w_i(Q_i) = a_i$$

and

$$b = -\Lambda a,$$

where $a = \mathrm{col}\{a_1, a_2, a_3\},\ b = \mathrm{col}\{b_1, b_2, b_3\},\ b_i = \dfrac{dw_i}{dx}(0) = \dfrac{dw_i}{dx}(Q_i).$

Proposition 1

If we know the exact solution w_a for the Dirichlet problem on the graph G_ε with the polynomials on the edges, it follows that the associated energy for such a solution takes the form $a(w_a, w_a) = -a^\top \Lambda_\varepsilon \cdot a$, thus the energy functional for the graph G reads

$$\phi \mapsto a(\Omega; \phi, \phi) = a(\Omega^0; \phi, \phi) - \phi(L-1)^\top \Lambda_\varepsilon \cdot \phi(L-1).$$

Remark 3.1

Λ_ε is negative semidefinite because with the identical Dirichlet conditions, the solution is constant so the energy is zero.

- The model defined on G_ε is $-w_i'' = 0$ on $E_{\varepsilon,i}$.
- The solutions on $E_{\varepsilon,i} = [0, L_{\varepsilon,i}]$ are given by

$$w_i(x) = \alpha_i x + \beta_i, x \in [0, L_{\varepsilon,i}] .$$

So $a_i = w_i(0) = \beta_i, b_i = \dfrac{dw_i(0)}{dx} = \alpha_i,\ b = \Lambda_\varepsilon a \Longleftrightarrow \alpha = \Lambda_\varepsilon \beta$.

- Considering the Kirchroff and continuity at P_4, P_5, P_6 respectively, we have

$$\begin{aligned}
(1-\varepsilon)\alpha_1 + \beta_1 &= \varepsilon\alpha_4 + (1-\varepsilon)\alpha_3 + \beta_3, \alpha_1 + \alpha_4 - \alpha_5 = 0, \\
(1-\varepsilon)\alpha_2 + \beta_2 &= \varepsilon\alpha_5 + (1-\varepsilon)\alpha_1 + \beta_1, \alpha_2 + \alpha_5 - \alpha_6 = 0, \\
(1-\varepsilon)\alpha_3 + \beta_3 &= \varepsilon\alpha_6 + (1-\varepsilon)\alpha_2 + \beta_2, \alpha_3 + \alpha_6 - \alpha_4 = 0.
\end{aligned} \tag{18}$$

$\Longrightarrow$

$$\Lambda_\varepsilon = \frac{1}{2\varepsilon - 3} \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}. \tag{19}$$

- The cost functional:

$$J(u) = \frac{1}{2}\sum_{i=1}^{3}\int_0^{L_i-1}(y_i - z_i)^2 + \frac{1}{2}|u-\zeta|^2 \,.$$

- Optimality system

$$\begin{cases} \sum_{i=1}^{3}\int_0^{L_i-1} y_i\phi_i + a(\Omega^0; p, \phi) - p(L-1)^\top \Lambda_\varepsilon \phi(L-1) = \sum_{i=1}^{3}\int_0^{L_i-1} z_i\phi_i, \\ a(\Omega^0; y, \phi) - p_1(0)\phi_1(0) - y(L-1)^\top \Lambda_\varepsilon \phi(L-1) = -\zeta\phi_1(0). \end{cases}$$

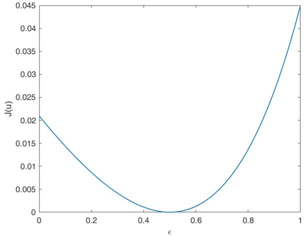

Fig. 7: The shape functional for $\varepsilon \in [0,1]$

Topological derivative

- $\dot{y}$: The derivative of $\varepsilon \to y$
- The topological derivative of cost functional:

$$\dot{J(u)} = \sum_{i=1}^{3} \int_0^{L_i-1} (y_i - z_i)\dot{y}_i + (u - \zeta)\dot{u}\,.$$

- The derivative with respect to ε of optimality system

$$\begin{cases} \sum_{i=1}^{3} \int_0^{L_i-1} \dot{y}_i\phi_i + a(\Omega^0; \dot{p}, \phi) - \dot{p}(L-1)^\top \Lambda_\varepsilon \phi(L-1) = p(L-1)^\top \dot{\Lambda}_\varepsilon \phi(L-1), \\ a(\Omega^0; \dot{y}, \phi) - \dot{p}_1(0)\phi_1(0) - \dot{y}(L-1)^\top \Lambda_\varepsilon \phi(L-1) = y(L-1)^\top \dot{\Lambda}_\varepsilon \phi(L-1). \end{cases}$$

Reference

- A.A. Novotny, J. Sokolowski, Topological derivatives in shape optimization. Springer Science Business Media, 2012.
- A.A. Novotny, J. Sokolowski, A. Zochowski, Applications of the topological derivative method. Springer, 2019.
- J. Sokolowski, A. Zochowski, Shape and topology optimization of distributed parameter systems. Control Cybernet. 42, no. 1, pp. 217–226, 2013. 2697-2718.
- A. Kowalewski, I. Lasiecka, J. Sokolowski, Sensitivity analysis of hyperbolic optimal control problems. Comput. Optim. Appl. vol. 52, no. 1, pp. 147-179, 2012.

Conclusion and Future

- Conclusion
  - Bilevel optimization problems
    - lower level: an optimal control problem
    - higher level: a shape and topology optimization problem
  - Domain decomposition technique:
    - Poincaré-Steklov operator
    - $G = G^0 \cup G_\varepsilon$
  - Topological derivative
- Future
  - Nonlinear state equation on metric graphs

Thank you for your attention!

谢谢聆听!